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R. E. Rudd

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PLASTICITY AND FAILURE IN NANOCRYSTALLINE BCC METALS VIA MOLECULAR DYNAMICS SIMULATION

Robert E. Rudd
Lawrence Livermore National Laboratory
Condensed Matter and Materials Division, L-045
Livermore, CA 94550-9698 USA
robert.rudd@llnl.gov

ABSTRACT

Advances in the ability to generate extremely high pressures in dynamic experiments such as at the National Ignition Facility has motivated the need for special materials optimized for those conditions as well as ways to probe the response of these materials as they are deformed. We need to develop a much deeper understanding of the behavior of materials subjected to high pressure, especially the effect of rate at the extremely high rates encountered in those experiments. Here we use large-scale molecular dynamics (MD) simulations of the high-rate deformation of nanocrystalline tantalum at pressures less than 100 GPa to investigate the processes associated with plastic deformation for strains up to 100%. We focus on 3D polycrystalline systems with typical grain sizes of 10-20 nm. We also study a rapidly quenched liquid (amorphous solid) tantalum. We apply a constant volume (isochoric), constant temperature (isothermal) shear deformation over a range of strain rates, and compute the resulting stress-strain curves to large strains for both uniaxial and biaxial compression. We study the rate dependence and identify plastic deformation mechanisms. The identification of the mechanisms is facilitated through a novel technique that computes the local grain orientation, returning it as a quaternion for each atom. This analysis technique is robust and fast, and has been used to compute the orientations on the fly during our parallel MD simulations on supercomputers. We find both dislocation and twinning processes are important, and they interact in the weak strain hardening in these extremely fine-grained microstructures. We also present some results on void growth in nanocrystalline BCC metals under tension.

INTRODUCTION

Metals with ultrafine (nanoscale) grain sizes are of considerable interest because of their mechanical properties as well as potentially advantageous performance in applications for which their ubiquitous grain boundaries can have a beneficial effect, such as in their response to radiation damage. The strength of polycrystalline materials increases with reducing grain size according to the Hall-Petch effect. One example where this increased strength can be beneficial is in fuel capsules for inertial confinement fusion (ICF). [1] The high strength allows capsules to contain high pressure fuel without rupture. In applications such as this, it is not only the static strength that is of interest, but the dynamic strength as well. Material strength resists the formation of hydrodynamic instabilities as the ICF capsule is compressed by powerful laser beams. Here we consider the dynamic strength of nanocrystalline tantalum at high rates and moderate pressures ($\sim$2 GPa) using molecular dynamics (MD) simulation [3, 2]. Since MD explicitly models the motion of atoms, it is possible to determine the strength (stress-strain behavior) and at the same time analyze the nucleation and flow of lattice defects including dislocations and deformation twins. We report the nature of these processes, as well as their strain rate dependence.

METHODS

We have used the MD code FEMD for these simulations. It is a concurrent finite element - molecular dynamics code which we used purely in MD. The details of the simulation technique are given in Ref. [3]. Simulations were run on 256-4096 CPUs of Opteron-based supercomputers.

In addition to integrating the equations of motion (F=ma) and calculating the thermodynamic properties (pressure, shear stress, temperature, etc.), the code also analyzes defects on the fly and calculates the lattice orientation for each atom. The technique for calculating the orientation is given in Ref. [3]. An example of the result is shown in Fig. 1. In the figure the nanoscale

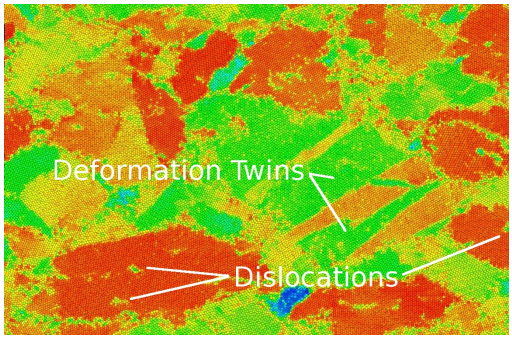

FIGURE 1. A slice through the 3D MD simulation box showing atoms colored according to the local lattice orientation after a strain of ∼20%. Different grains appear as different colors. Dislocations and deformation twins contributing to the plastic flow are indicated. [3]

grain structure is clearly identified by color, and local variations of the color indicate the local orientation changes due to dislocations. We have movies showing the propagation of the dislocation from the point of their nucleation at a grain boundary, through their glide across the grain to the point that they are absorbed into the grain boundary on the far side.

RESULTS

Some of the stress-strain curves from uniaxial isochoric (volume-conserving) deformation simulations at fixed strain rates are shown in Fig. 2. There is an initial elastic region, followed by incipient plasticity as the stress-strain curve deviates from the elastic curve. Then the shear stress peaks as sufficient plastic flow takes place to compensate the applied deformation rate. Then the shear stress relaxes due to further plastic flow. Eventually, the shear stress reaches a plateau, even increasing at a low rate of strain hardening due to further evolution of the microstructure. During the deformation, both dislocation activity and deformation twinning contribute to the plastic flow. Dislocation activity leads to pronounced grain rotations and in some cases grain coalescence, and deformation twinning further refines the microstructure.

The peak in the shear stress increases with increasing strain rate. This effect is important for several reasons. [3] One example is that the high shear stresses at high rates can lead to the activation of processes that do not occur at lower rates. The steep increase in shear stress at the high strain rates shown in Fig. 3 cautions against running MD at the less demanding higher strain rates whereas below $\dot{\varepsilon} = 3 \times 10^8$/s the stress is reasonably constant.

CONCLUSIONS

We have conducted MD simulations of the deformation of nanocrystalline tantalum at moderate pressures and high rates. We have found a pronounced strain-rate effect at high rates, and have analyzed the associated mechanisms of plasticity.

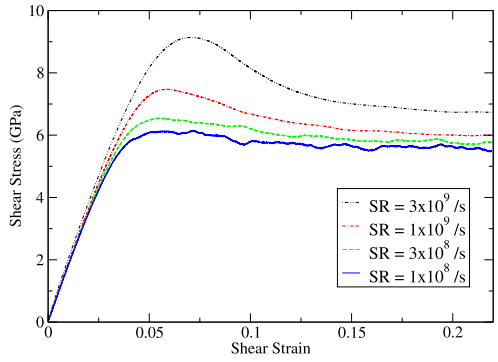

FIGURE 2. Stress-strain curves for nanocrystalline Ta as simulated in MD at four strain rates: $\dot{\varepsilon} = 3 \times 10^9, 10^9, 3 \times 10^8, 10^8$/s. The simulation at $\dot{\varepsilon} = 10^9$/s continued to a total strain greater than unity, but those results are not shown here. [3]

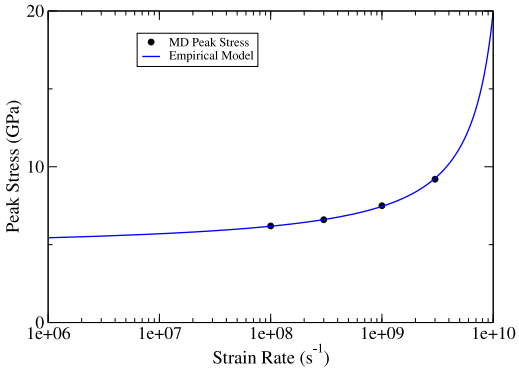

FIGURE 3. Peak shear stress as a function of strain rate. [3]

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